

Nitromethane  
75-52-5 | DTXSID2020977

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

## Model Results

**Predicted value:** -0.468

**Global applicability domain:** Inside

**Local applicability domain index:** 5.64e-01

**Confidence level:** 7.44e-01

## Nearest Neighbors from the Training Set

Image not found

Nitromethane

**Measured:** -0.350

**Predicted:** -0.468

Image not found

Formamide

**Measured:** -1.51

**Predicted:** -1.32

Image not found

Formic acid

**Measured:** -0.540

**Predicted:** -0.578

Image not found

Methyl carbamate

**Measured:** -0.660

**Predicted:** -0.611

Image not found

Acetaldehyde oxime

**Measured:** -0.130

**Predicted:** 2.71e-01